

## Study of dispersion relations based on a five parameter model

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The lattice dynamics of fcc transition metals has been discussed on the basis of a five parameter model. Three radial for first, second and third neighbours and one angular parameter for first neighbour have been employed to express the ion-ion interactions. The electron-ion interactions have been considered on the basis of modified Cheveau scheme.

The dispersion relations for nickel and platinum have been computed on the basis of the model. Theoretical predictions have been found to be in good agreement with the experimental data.

### 1 INTRODUCTION

Various authors (Kulshrestha & Upadhyay 1976, Upadhyaya *et al* 1975, Singh *et al* 1975, Bertolo & Shukla 1975, Goel *et al* 1974, Prakash *et al* 1975, Bakshi & Tripathi 1972, 1970) have discussed the lattice dynamics of transition metals. Some of these studies make use of de-Launay (1956) type of angular interactions which are rotationally invariant. The others use Sharma-Joshi (1963) type volume interactions which are asymmetric (Lax 1963) in the reciprocal space. The Krebs (1965) electron ion interaction used by Kulshrestha & Upadhyaya (1976) suffer from the deficiency of internal-equilibrium (Cochran 1968). The Bhatia (1955) model used by Bertolo & Shukla (1975) is also deficient in these regards.

The experiments on inelastic scattering of slow neutrons show that the interatomic forces are of fairly long-range nature in transition metals. The overlapping of core and incomplete electronic shells, responsible for large cohesive energy in transition metals impress upon the existence of moderately long range forces. The part of Cauchy's discrepancy and the anisotropy exhibited by these metals suggest the presence of many body forces which could be accounted for in terms of ionic angular interactions. In view of these facts a new model has been developed. The most significant ion-ion interactions have been assumed to be radial upto third neighbours and the Clark *et al* (1964) type angular forces for first neighbours only. The volume interactions as reported by Cheveau (1968) have been modified to take into account (a) the reduction of effective potential at the core region (b) the actual nature of the electron wave function, (c) the repulsion due to electrons and (d) the wave number dependence of screening parameter. The model is used to compute the phonon-frequencies for nickel and platinum.

## 2 THEORY AND RESULTS

The following secular determinant is used to express the phonon-frequencies ( $\nu$ )

$$|D - 4\pi^2 m \nu^2 I| = 0 \quad \dots (1)$$

where  $m$  is the mass of the atom and  $I$  is the unit matrix of the order three. The diagonal and off-diagonal matrix elements  $[D]$  are the sum of ion-ion  $[D_{\alpha\beta}^I]$  terms and electron-ion  $[D_{\alpha\beta}^E]$  terms

The ion-ion terms  $[D_{\alpha\beta}^I]$  for fcc structure are expressed as

$$\begin{aligned} D_{\alpha\beta}^I &= (2\alpha_1 - 16y)S_\alpha S_\beta + 4/3 S_\alpha S_\beta \alpha_3 [4Cy(C'_\alpha + C'_\beta) - (1 - 2Cy)^2] \\ D_{\alpha\alpha}^I &= 2[\alpha_1 + 8y][2 - C'_\alpha(C_\beta + Cy)] + 4\alpha_2 S_\alpha^2 + \frac{16}{3}[1 + C_\beta Cy(1 - 2C_\alpha^2)]\alpha_3 \\ &\quad + 8/3\alpha_3 \left[ 1 + \frac{C_\alpha}{2}(C_\beta + Cy)(1 - 2C_\beta Cy) \right] - 4y(2C'_\alpha - C'_\beta - C'y) \end{aligned} \quad \dots (2)$$

where  $\alpha, \beta = 1, 2, 3$ ,  $S_\alpha = \sin(\frac{1}{2}aq\alpha)$ ,  $C'_\alpha = \cos(\frac{1}{2}aq\alpha)$ ,  $C''_\alpha = \cos(aq\alpha)$ ,  $\alpha_1, \alpha_2, \alpha_3$  are the radial force constants for the first, second and third neighbouring ions respectively,  $y$  is the angular force constant for the nearest neighbour,  $a$  is the lattice parameter and  $q\alpha$  is the  $\alpha$ -component of the wave vector  $q$

The electron-ion terms  $D^E$  can be written as

$$D_{\alpha\beta}^E = -\frac{e^2 \lambda^2}{4} K_F \sum_i \left[ \frac{(i + \ell)_\alpha (i + \ell)_\beta g^2(1q + \ell_1 \gamma_s)}{1q + \ell_1^2 + \lambda^2 f(\ell_1)} - \frac{\ell_\alpha \ell_\beta q^2 (1G) \gamma_s}{\ell_1^2 + \lambda^2 f(\ell_1)} \right] \quad (3)$$

where  $K_F$  is the bulk modulus of the electron gas. The equation (3) represents the modified form of Cheever (1968) expression. The Bardeen (1937) function  $g$  has been introduced to reduce the effective potential at the core region of the ions and to admit the Bloch type electron wave functions. These functions have been further modified on the line reported by Bross & Bohm (1967) and successfully applied by Goel *et al* (1975, 1974a, 1974b). The screening parameter ( $\lambda$ ) has been modified to take into account its dependence on wave number and the repulsion due to electrons. These modification suggested by Langer & Vosko (1959) and Pines (1955) lead to the modified screening parameter as

$$\lambda = 0.353 \left( \frac{r_0}{a_0} \right)^{\frac{1}{3}} K_F, \quad \dots (4)$$

where  $r_0$  = Inter electronic spacing =  $\gamma_s/Z^{1/3}$

$\gamma_s$  = radius of atomic sphere  $Z$  = valence

$\gamma_s$  = radius of atomic sphere

$a$  = Bohr radius,  $K_F$  = Radius of Fermi sphere

and

$$f(\ell) = \frac{1}{2} + \frac{1 - \ell^2}{4\ell} L_n \left( \frac{1 + \ell}{1 - \ell} \right), \ell_1 = \frac{1q + G}{2K_F}, \ell_2 = |G|/2K_F, \quad \dots (5)$$

The five model parameters ( $\alpha_1$ ,  $\alpha_2$ ,  $\alpha_3$ ,  $y$  and  $aKe$ ) have been computed independently making use of known value of three elastic constants ( $C_{11}$ ,  $C_{12}$ ,  $C_{44}$ ) and two zone boundary frequencies  $\nu_1$  and  $\nu_2$  of transverse modes along the direction [100] and [111] respectively. The resulting expressions are

$$\alpha_1 = 9/2(\pi^2 m \nu_1^2 - \frac{1}{2} aKe + \frac{1}{2} aC_{12} - \frac{23}{9} aC_{44}) \quad \dots (6)$$

$$\alpha_2 = \pi^2 m \nu_2^2 - \frac{1}{2} \pi^2 m \nu_1^2 - \frac{1}{2} (aKe - aC_{12} + aC_{44}) \quad \dots (7)$$

$$\alpha_3 = \frac{3}{4} (\frac{1}{2} aKe + \frac{3}{2} aC_{44} - \pi^2 m \nu_1^2 - \frac{1}{2} aC_{12}) \quad \dots (8)$$

$$y = \frac{1}{16} (aKe - aC_{12} + aC_{44}) \quad \dots (9)$$

$$aKe = aC_{11} - aC_{12} - aC_{44} - 4\pi^2 m \nu_1^2 + 2\pi^2 m \nu_2^2 \quad \dots (10)$$

The input data for nickel and platinum are given in table 1 and the computed model parameters are enlisted in table 2

Table 1 Input data

Nickel		Platinum	
Values	Reference	Values	Reference
$C_{11} = 2.508 \times 10^{12}$ dyn/cm <sup>2</sup>		$C_{11} = 3.467 \times 10^{12}$ dyn/cm <sup>2</sup>	
$C_{12} = 1.500 \times 10^{12}$ ..	Kittel (1971)	$C_{12} = 2.507 \times 10^{12}$ ..	MacFarlane <i>et al</i> (1965)
$C_{44} = 1.235 \times 10^{12}$ ..		$C_{44} = 0.765 \times 10^{12}$ ..	
$a = 3.524$ Å		$a = 3.92$ Å	
$m = 58.71$ amu		$m = 195.02$ amu	
$\nu_1 = 6.27 \times 10^{13}$ HZ		$\nu_1 = 3.84 \times 10^{13}$ HZ	
$\nu_2 = 4.24 \times 10^{13}$ HZ	Bingenau <i>et al</i> (1964)	$\nu_2 = 2.90 \times 10^{13}$ HZ	Dutton <i>et al</i> (1972)

Table 2 Model parameters

Nickel		Platinum	
$\alpha_1$	$37.13805 \times 10^4$ dyne/cm	$\alpha_1$	$39.11405 \times 10^4$ dyne/cm
$\alpha_2$	$1.02870 \times 10^4$ ..	$\alpha_2$	$6.19042 \times 10^4$ ..
$\alpha_3$	$-5.46434 \times 10^4$ ..	$\alpha_3$	$-6.16143 \times 10^4$ ..
$\gamma$	$-0.06729 \times 10^4$ ..	$\gamma$	$-0.37920 \times 10^4$ ..
$aKe$	$-0.14875 \times 10^4$ ..	$aKe$	$-0.72617 \times 10^4$ ..

The computed dispersion-curves for nickel and platinum are shown in figures 1 and 2 respectively. The experimental points (O $\Delta$  $\blacktriangle$ ) reported by Birgeneau *et al* (1964) and Dutton *et al* (1972) for nickel and platinum respectively, closely follow the theoretical curves. The deviations which are less than 3% particularly at zone boundaries, loses their significance when compared to the experimental errors creeping into the measurement of phonon frequencies.

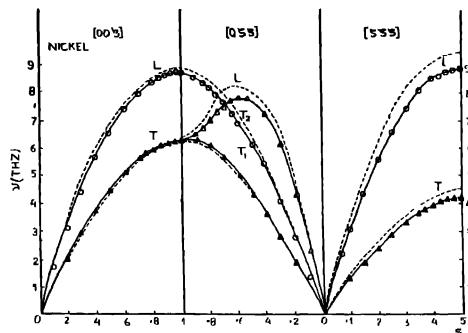


Fig. 1. Dispersion Curves for Nickel

[ — theoretical (author) O.  $\Delta$ .  $\blacktriangle$  Experimental (Birgeneau *et al* (1964)) - - - theoretical (Behari & Tripathi (1970)),

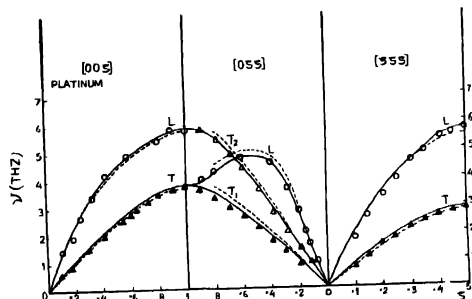


Fig. 2. Dispersion Curves for Platinum

[ — theoretical (author) O.  $\Delta$ .  $\blacktriangle$  Experimental (Dutton *et al* (1972)) - - - theoretical (Goel *et al* (1974a))),

### 3 DISCUSSION

The dispersion curves (shown by continuous lines in figures) computed on the basis of the present model are compared with those (shown by dotted lines

in figures) of Goel *et al* (1974a) and Behari & Tripathi (1970) for platinum and nickel respectively. The theoretical curves of these studies show marked deviations ( $L$  and  $T$  branches along  $[111]$  and  $[110]$  directions) at zone boundaries. This could be attributed to the inherent drawback of Sharma-Joshi (1963) scheme.

The close agreement between the computed and experimental data could be inferred as the success of the present study in describing the possible interactions governing the lattice-vibrations of transition-metals (fcc).

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